

Phase Diagram of the Interacting Lieb-Kitaev chain model

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We study an interacting spinless Lieb-Kitaev chain in the nearly flat-band regime, motivated by the recent observation that Majorana zero modes in the non-interacting Lieb-Kitaev system inherit two decay modes: an ordinary Bogoliubov-de Gennes localization length and a longer geometric length controlled by the quantum metric. Using finite-system density-matrix renormalization group (DMRG) calculations, we analyze how these structures evolve under repulsive nearest-neighbor density interaction. At weak coupling the data remain compatible with a surviving long geometric Majorana scale, whereas at larger repulsion the system exhibits charge order, showing repeated transitions between commensurate and incommensurate CDW phases, and a conventional density-ordered phase in the strong coupling regime. These results support the view that in flat-band topological superconductors quantum geometry and interaction-driven ordering are deeply intertwined.

I. INTRODUCTION

Over the past two decades, flat-band materials have attracted considerable interest. Owing to the quenching of kinetic energy in flat bands, interaction effects are substantially enhanced and can dominate the low-energy physics, rendering flat-band systems a fertile platform for investigating strongly correlated phenomena and interaction-driven quantum phases. This has led to the realization of a wide range of exotic states, including unconventional superconductivity [1–3], magnetism [4, 5], and fractional topological phases [6–8].

For a superconducting (SC) phase within a conventional single-band BCS picture, a perfectly flat band has vanishing band curvature and thus an infinite effective mass would appear to strongly inhibit superconductivity. In contrast, in multiband flat-band systems, the complete quenching of the band dispersion does not eliminate the nontrivial momentum-space structure of the Bloch wave functions [9–12]. The Bloch states can retain a finite extent in Hilbert space across the Brillouin zone, reflecting their variation with crystal momentum, and this quadratic spread is quantified by the quantum metric through the infinitesimal distance between neighboring Bloch states [13–15]. Such nontrivial quantum geometry provides an additional channel for superconducting transport that is absent in the conventional single-band picture. As a consequence, a finite superfluid weight and robust superconducting coherence can persist even in the flat-band limit, despite the absence of conventional band-dispersion contributions [2, 16–18].

The superconducting coherence length is a fundamental length scale that characterizes the spatial extent of

superconducting correlations. In conventional BCS superconductors, it is given by $\xi_{\text{BCS}} \sim \hbar v_F / \Delta$, where v_F is the Fermi velocity and Δ is the pairing gap. This length scale measures the characteristic size of Cooper pairs. By comparison, recent developments have shown that the quantum metric of Bloch wave functions not only generates a finite geometric contribution to the superfluid weight, but also establishes an intrinsic length scale governing superconducting phenomena [19–21]. This geometric viewpoint became significant in the recent analysis of Majorana zero modes in the noninteracting Lieb-Kitaev model [22]. There, the edge mode does not exhibit a single localization length. Instead, one finds two distinct correlation lengths: a short Bogoliubov-de Gennes scale associated with ordinary topological superconducting localization [23, 24], and a longer geometric scale inherited from the spread of flat-band wave functions. The latter is controlled by the quantum metric and can become parametrically large in the nearly flat-band regime. This immediately raises a many-body question: once repulsive interactions are introduced, does the geometric long tail survive as a physically meaningful scale, or is it washed out by correlation-driven reconstruction?

In previous studies, interactions were typically introduced in the form of an attractive pairing channel, which directly promotes Cooper pairing and thereby induces superconductivity. Representative examples in one dimension include stub [25], sawtooth [26], Creutz [12, 26–28], and related multiorbital chains. Here, we retain the attractive interaction responsible for superconducting pairing while introducing a repulsive interaction to incorporate competing correlation effects beyond the pairing channel. Such a coexistence of attractive and repulsive interactions is physically natural in many electronic systems: an effective attractive pairing interaction may arise from phonons, collective fluctuations, or superexchange processes, while residual Coulomb interactions remain repulsive. This situation is encountered, for exam-

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ple, in electron-phonon superconductors [29, 30], moiré flat-band systems [31, 32], and extended Hubbard models [33, 34], where the competition between pairing and repulsion can substantially reshape the superconducting state and stabilize competing charge-ordered phases.

To address this question beyond mean-field theory, we employ density-matrix renormalization group (DMRG) calculations to investigate the interacting one-dimensional flat-band superconductor. By systematically resolving its phase structure, correlation functions, and characteristic length scales, we aim to determine how repulsive interactions reshape superconductivity and whether the quantum-geometric length scale remains robust in the many-body regime.

II. MODEL AND THEORETICAL FRAMEWORK

We consider an interacting Lieb–Kitaev chain model, governed by the Hamiltonian.

$$H = H_0 + H_U, \quad (1)$$

with

$$\begin{aligned} H_0 = & -t \sum_j \sum_{\alpha=A,B,C} \left(c_{j\alpha}^\dagger c_{j+1,\alpha} + \text{h.c.} \right) \\ & - V \sum_j c_{jA}^\dagger c_{jA} + V \sum_j c_{jC}^\dagger c_{jC} \\ & - J \sum_j \left(c_{jA}^\dagger c_{jB} + c_{jC}^\dagger c_{jB} + \text{h.c.} \right) \\ & - J \sum_j \left(c_{jA}^\dagger c_{j+1,B} + c_{jC}^\dagger c_{j+1,B} + \text{h.c.} \right) \\ & + \Delta \sum_j \sum_{\alpha=A,B,C} (c_{j\alpha} c_{j+1,\alpha} + \text{h.c.}). \end{aligned} \quad (2)$$

and

$$H_U = U \sum_{j=1}^{L-1} \sum_{\alpha=A,B,C} \left(\hat{n}_{j\alpha} - \frac{1}{2} \right) \left(\hat{n}_{j+1,\alpha} - \frac{1}{2} \right) \quad (3)$$

The Lieb–Kitaev model describes a one-dimensional three-orbital lattice at open boundary condition with orbitals A , B , and C in each unit cell j (Fig. 1(a)). We denote the number of unit cells by L and the total number of orbitals by $N = 3L$. The onsite energies of the three orbitals are shifted by $-V$, 0 , and $+V$. The hopping amplitude J couples the B orbital to the neighboring A and C orbitals, both within the same unit cell and between adjacent unit cells, forming the characteristic Lieb-like lattice geometry. To realize a topological superconducting phase, nearest-neighbor intra-orbital pairing

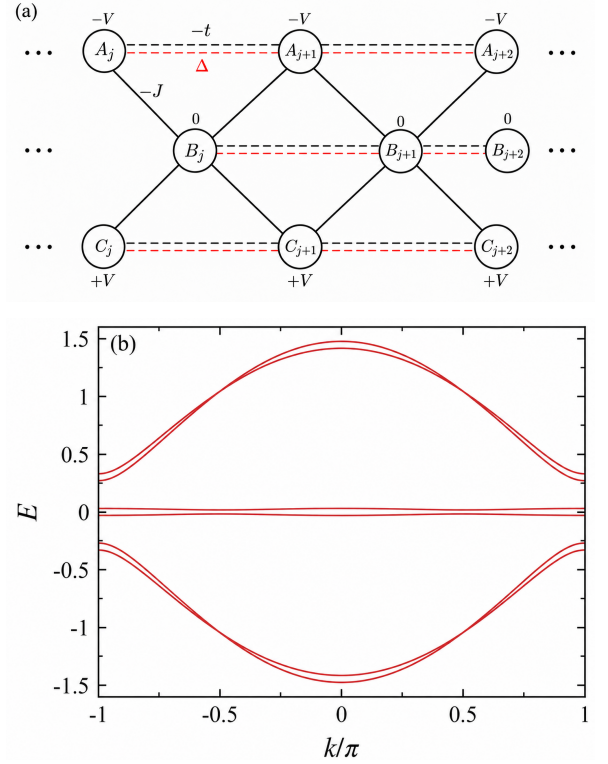


FIG. 1. (a): Lattice structure of the Lieb–Kitaev chain. (b): Energy bands of the one-dimensional Lieb–Kitaev chain model for $t = 0.03$, $V = 0.6$, $J = 1$, and $\Delta = 0.018$.

with amplitude Δ is introduced between the same orbitals in adjacent unit cells. In addition, a weaker hopping t connects identical orbitals in neighboring unit cells and gives the otherwise flat middle band a small dispersion: $\epsilon_0 = -2t \cos(ka)$, where a is the unit cell spacing.

To maintain the flat-band regime, the dispersion of the middle band, characterized by the energy scale $2t$, should be much smaller than the separation from the dispersive bands, $E_g = |V|$ and the dominant hopping J . When we choose parameters $t = 0.03$, $V = 0.6$, $J = 1$, $\Delta = 0.018$, the flat-band condition remains satisfied (Fig. 1(b)).

Recent work [22] showed that the Majorana edge profile in the Lieb–Kitaev model inherits both a short localization length and a longer scale tied to ξ_{QM} . For the noninteracting parent model, the bulk property given by Bloch states $|u_n(k)\rangle$ define the quantum geometric tensor

$$\mathcal{Q}_{\mu\nu}(k) = \langle \partial_\mu u(k) | [1 - |u(k)\rangle\langle u(k)|] | \partial_\nu u(k) \rangle, \quad (4)$$

Solving the Hamiltonian in momentum space, the eigenstate of the middle band can be written as

$$|u_0(k)\rangle = \frac{1}{\sqrt{4J^2[1 + \cos(ka)] + V^2}} \begin{pmatrix} a_k \\ V \\ -a_k \end{pmatrix} \quad (5)$$

where $a_k = -J(1 + e^{ika})$. We define the quantum metric length through the Brillouin-zone-averaged quantum metric

$$\xi_{\text{QM}} \equiv \frac{1}{a} \frac{a}{2\pi} \int_{\text{BZ}} dk \mathcal{Q}_{\mu\nu}(k) \simeq \frac{\sqrt{2}}{4} \frac{J}{V} a \quad (6)$$

On the other hand, the Majorana wave function under open boundary conditions can be constructed from the projected bulk Green's function,

$$\psi_L(x) \propto G^p(x, x_L; 0) \chi_L, \quad (7)$$

where

$$G^p(x, x'; 0) = \sum_{n=\pm} \int \frac{dk}{2\pi} \frac{g_n(k) g_n^\dagger(k)}{-\epsilon_n(k)} e^{ik(x-x')}. \quad (8)$$

where $\epsilon_n(k)$ denotes the dispersion of the two low-energy Bogoliubov quasiparticle bands, while $g_n(k)$ is the corresponding BdG Bloch eigenstate. The vector χ_L encodes the local boundary coupling that generates the left Majorana mode under open boundary conditions.

The low-energy BdG eigenstates can be factorized as

$$g_\pm(k) = v_\pm(k) \otimes u_0(k), \quad (9)$$

Here, $v_\pm(k)$ describes the particle-hole structure of the effective Kitaev sector, whereas $u_0(k)$ is the Bloch eigenstate of the normal-state flat band and describes its orbital structure. Accordingly, the projected Green's function contains two distinct momentum-dependent factors. The quasiparticle part, consisting of $v_\pm(k) v_\pm^\dagger(k)$ together with $1/\epsilon_\pm(k)$, produces poles associated with the BdG quasiparticle dispersion and gives the conventional localization length ξ_{BCS} . In contrast, the orbital projector $u_0(k) u_0^\dagger(k)$ contains additional poles originating from the momentum dependence of the flat-band Bloch wave function. These poles generate the geometric localization length that is just $4\xi_{\text{QM}} = \frac{\sqrt{2}J}{V} a$. Consequently, the Majorana wave function contains two exponentially decaying components,

$$\psi_L(x) = A_{\text{BCS}} e^{-x/\xi_{\text{BCS}}} + A_{\text{QM}} e^{-x/(4\xi_{\text{QM}})}. \quad (10)$$

III. NUMERICAL STRATEGY

The interacting ground state is computed by finite-system DMRG with open boundary conditions using ITensor [35]. The three-orbital chain is mapped to a one-dimensional matrix-product-state sequence $(A_1, B_1, C_1, A_2, B_2, C_2, \dots, A_L, B_L, C_L)$. We choose the parameter $t = 0.03$, $V = 0.6$, $J = 1$ and $\Delta = 0.018$ and restrict the system to half filling for this spinless model. The source calculations emphasize careful sweep scheduling and convergence control, which is essential because the entanglement rises substantially in parts of the repulsive regime and because flat-band systems generally exhibit a large degree of degeneracy. Each parameter point

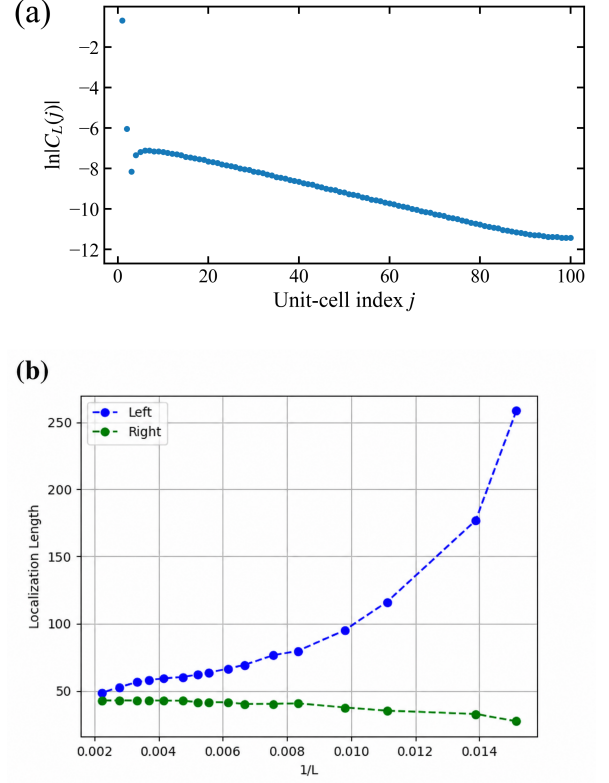


FIG. 2. (a) Logarithmic boundary-correlation profile $C_L(j) = \langle c_{jB} \gamma_L \rangle$, with $\gamma_L = c_{1B} + c_{1B}^\dagger$, for $N = 300$ orbital sites. Here j labels unit cells. The rapid variation near the boundary is followed by a more slowly decaying tail. (b) Decay lengths extracted from the left-boundary (blue) and right-boundary (green) correlation profiles as functions of the inverse system size $1/L$. The parameters are $t = 0.03$, $V = 0.1$, $J = 1$, and $\Delta = 0.018$. With $a = 3$, the geometric reference scale is $4\xi_{\text{QM}} \simeq \sqrt{2}Ja/V \approx 42.4$.

is initialized independently from the empty-site product state and optimized through a prescribed sequence of 80 full sweeps. The maximum bond dimension is increased progressively through 20, 40, 80, 160, 320, 640, and 1280, while the truncation cutoff is tightened from 10^{-4} through 10^{-6} and 10^{-8} . A density-matrix noise term is included during the initial optimization, with its coefficient gradually reduced from 10^{-5} to 10^{-10} . A custom observer records the total energy and the von Neumann entanglement entropy after every full sweep. Convergence is assessed by requiring both the absolute change in the total energy and the maximum change in the entanglement entropy over all intercell cuts between the final two sweeps to be smaller than 10^{-7} .

The nontrivial decay modes in this model can be characterized by the superconducting coherence length, which is conventionally extracted from the pair correlation function and remains applicable in flat-band systems. Here we adopt an alternative approach based on the geometric character of the flat band. In this case, the relevant superconducting length scale is related to the

U	0–0.1	0.1–0.3	0.3–0.8	0.8–2.5	> 2.5
Charge sector	TC (B)	ICDW (A, B, C)	CDW (A, C)	CDW (A, C) ICDW (B)	CDW (A, B, C)
Bond order	—	IBOW (A, B, C)	BOW (B)	BOW (B)	BOW (A, C)
Pairing modulation	—	IPDW (A, B, C)	PDW (B)	PDW (B)	—
Central charge c	0	≈ 1	0	≈ 1	0

TABLE I. Finite-size phase diagram of the interacting Lieb–Kitaev chain in different interaction regimes. (ABC) specify the corresponding orbitals. CDW, BOW, and PDW denote charge-density wave, bond-order wave, and pair-density wave, and ICDW refers to an incommensurate phase, respectively. The parameters are $t = 0.03$, $\Delta = 0.018$, $V = 0.6$, and $J = 1$. Charge sector is measured with $\langle \hat{n}_i \rangle$, Bond order is measured with $\langle c_{i\alpha}^\dagger c_{i+1\alpha} \rangle$, pairing order is measured with $\langle c_{i\alpha} c_{i+1\alpha} \rangle$. The boundaries between the listed regimes are approximate.

quadratic spread of the Wannier states, which is governed by the Bloch functions and can be directly accessed through single-particle correlation functions $\langle c_i^\dagger c_j \rangle$, $\langle c_i c_j \rangle$. (Fig. 2) shows the two exponential decay modes of the correlation function, with a decay length nearly independent of the reference position in the bulk, together with the finite-size dependence of the decay lengths extracted from correlations anchored at either end of the chain. These quantities can be used to characterize the long-range collective decay modes, and after extrapolation to the thermodynamic limit, the extracted values are consistent with the theoretical predictions.

We use the central charge to justify an ICDW phase. In one dimension, the ICDW phase is typically gapless and is described by a Luttinger liquid, so the entanglement entropy follows the conformal scaling form with a finite central charge, usually $c = 1$ for a single gapless charge mode. By contrast, a commensurate CDW phase is generally gapped, for which the entanglement entropy saturates at long distances and the effective central charge vanishes, $c = 0$. A fully gapped one-dimensional superconducting phase, including a gapped topological superconducting phase, has no gapless bulk degrees of freedom and therefore corresponds to an effective central charge $c = 0$. The central charge can be obtained from entanglement entropy with the Calabrese–Cardy formula at open boundary condition [36].

$$S(\ell) = \frac{c}{6} \ln \left[\frac{2L}{\pi} \sin \left(\frac{\pi \ell}{L} \right) \right] + s_0. \quad (11)$$

IV. RESULTS

Our finite-size DMRG calculations are consistent with a rich interaction-driven sequence of regimes in the half-filled interacting Lieb–Kitaev chain. The finite-size DMRG data are summarized in Table I. Starting from weak interactions, the system first remains in the gapped topological superconducting phase continuously connected to the noninteracting Lieb–Kitaev limit, where

the quantum-metric-induced length scale remains visible in the long-distance single-particle correlations. Upon increasing the nearest-neighbor repulsion U , the system enters an incommensurate charge-density-wave (ICDW) regime for approximately $0.1 \lesssim U \lesssim 0.3$, characterized by spatially modulated charge correlations and a finite central charge $c \simeq 1$, indicating a gapless Luttinger-liquid-like mode. This is followed by a reentrant gapped topological regime for $0.3 \lesssim U \lesssim 0.8$, with a vanishing central charge and saturated entanglement entropy. At stronger interactions, another gapless ICDW regime emerges for $0.8 \lesssim U \lesssim 2.5$, again accompanied by $c \simeq 1$, before the system finally evolves into a strongly coupled commensurate CDW phase for $U \gtrsim 2.5$, where the charge density becomes locked into a period-two pattern and the central charge returns to $c = 0$. In the intermediate regimes, the charge modulations are accompanied by corresponding bond- and pair-density modulations, reflecting the strongly intertwined charge, bond, and superconducting correlations of the multiorbital flat-band system.

This evolution is most directly visualized through $n_\alpha(i)$. At weak coupling, the density is spatially uniform within each orbital, although the average occupations of different orbitals need not coincide. Incommensurate modulations subsequently develop on all three orbitals, producing an ABC -ICDW pattern. With increasing interaction, the A and C densities lock into pronounced period-two CDW configurations, while the B density becomes nearly uniform again. The next regime retains this commensurate AC background, but the B orbital develops a renewed incommensurate density response. Finally, the B density also locks into a period-two pattern as its average occupation approaches half filling, completing the formation of an ABC -CDW state. The B orbital thus undergoes a distinctive sequence of modulation, flat-tening, and renewed modulation before joining the final commensurate state.

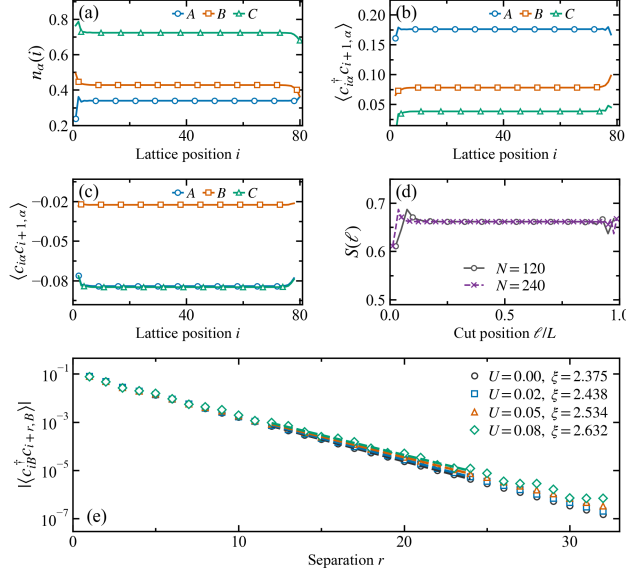


FIG. 3. Weak-interaction TC regime for (a)–(c) Orbital-resolved density, normal bond expectation value, and pairing expectation value at $U = 0.05$ and $N = 240$. Colors and symbols identify $\alpha = A, B, C$, and i counts unit cells. (d) Entanglement entropy for $N = 120, 240$, with $L = N/3$. (e) Magnitude of the normal correlation $\langle c_{iB}^\dagger c_{i+r,B} \rangle$ at $i = 40$, $N = 240$, and $U = 0, 0.02, 0.05, 0.08$; r is measured in unit cells.

A. Regime I: topological regime

The weak-interaction regime labelled TC ($0 \leq U \lesssim 0.1$) is characterized by spatially uniform bulk observables and a noncritical entanglement structure. (Fig. 3(a)–(c)) show representative results at $U = 0.05$ for $N = 240$. The normal bond expectation values $\langle c_{i\alpha}^\dagger c_{i+1,\alpha} \rangle$ and pairing expectation values $\langle c_{i\alpha} c_{i+1,\alpha} \rangle$ likewise approach uniform bulk values for $\alpha = A, B, C$. Thus, no bulk CDW, intraorbital BOW, or PDW modulation is resolved in these profiles. The nonzero, spatially uniform pairing amplitudes are compatible with the explicit pairing term in the Hamiltonian.

The entanglement entropy reaches an essentially size-independent plateau for $N = 120$ and 240 (Fig. 3(d)). Fitting the central half of the chain yields $c_{\text{eff}} \simeq 0$, consistent with a noncritical bulk. The normal correlation function on the B orbital,

$$G_B(r) = \langle c_{iB}^\dagger c_{i+r,B} \rangle, \quad i = 40, \quad (12)$$

exhibits approximately exponential decay (Fig. 3(e)) with $\xi \simeq 7.124, 7.314, 7.602, 7.897$ for $a = 3$ at $U = 0, 0.02, 0.05, 0.08$, respectively. The fitted decay length increases with interaction strength, while the approximately exponential form persists over the examined interval. Deviations from a single exponential become more visible at $U = 0.08$.

We therefore identify phase I as the topological refer-

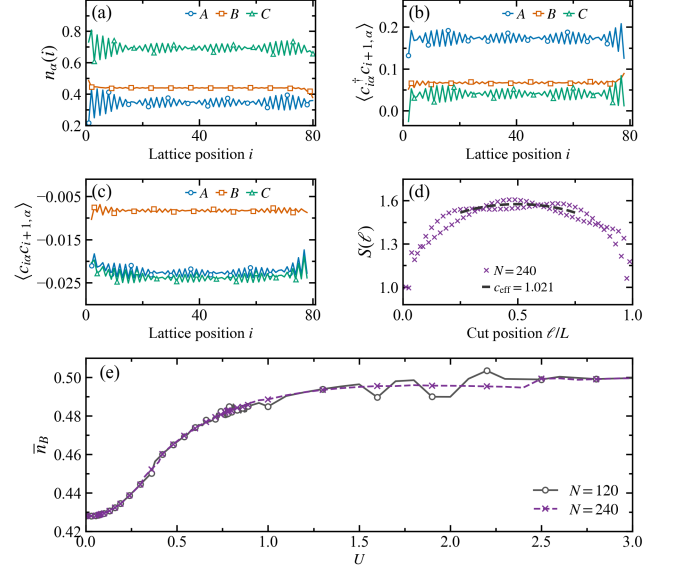


FIG. 4. Density, bond, pairing, and entanglement signatures of the ICDW regime. (a)–(c) $n_\alpha(i)$, $\langle c_{i\alpha}^\dagger c_{i+1,\alpha} \rangle$, and $\langle c_{i\alpha} c_{i+1,\alpha} \rangle$, respectively, at $U = 0.24$ and $N = 240$. Colors and symbols distinguish $\alpha = A, B, C$; i labels unit cells. (d) Entanglement entropy at $U = 0.24$ for $N = 240$, with $L = N/3 = 80$. The fitted coefficient is $c_{\text{eff}} = 1.021$; (e) Mean B -orbital occupation in the central half of the chain, $\bar{n}_B = (2/L) \sum_{i=L/4+1}^{3L/4} n_B(i)$, over $0 \leq U \leq 3$ for $N = 120, 240$.

ence state from which the interaction-driven reconstruction begins. The correlation function exhibits the smooth long-ranged structure expected for the topological parent state, while the entropy profile remains consistent with a gapped regime. The sublattice occupations are already unequal, but they do not yet show the pronounced interaction-driven incommensurate locking that appears at larger U .

B. Regime II: ICDW regime

The second regime develops simultaneous modulations of the density, bond expectation values, and pairing amplitudes. At $U = 0.24$, the orbital-resolved profiles in (Fig. 4(a)–(c)) display spatial oscillations with a slowly varying envelope, in contrast to the uniform bulk profiles of the TC regime. Corresponding oscillations occur in both $\langle c_{i\alpha}^\dagger c_{i+1,\alpha} \rangle$ and $\langle c_{i\alpha} c_{i+1,\alpha} \rangle$ for $\alpha = A, B, C$, identifying coupled density, bond, and pairing modulations on the finite chains. Moreover, the dominant Fourier component of each mean-subtracted bulk profile occurs at the same resolved wave vector, $Q \simeq 0.95\pi$, with the unit-cell spacing set to unity. This common component, displaced from the period-two value $Q = \pi$, supports an ABC charge modulation with incommensurate character on the studied finite chain.

For $N = 240$, the entanglement entropy exhibits oscillations about a smooth profile (Fig. 4(d)). We estimate the effective central charge. A fit over $L/4 \leq \ell \leq 3L/4$ yields $c_{\text{eff}} = 1.021$ for $N = 240$. These estimates are compatible with a $c \simeq 1$ critical regime.

The mean occupation of the B orbital provides a complementary measure of the interaction-driven density redistribution. Defining a bulk average over the central half of the chain, $\bar{n}_B = \frac{2}{L} \sum_{i=L/4+1}^{3L/4} \langle c_{iB}^\dagger c_{iB} \rangle$ we plot its evolution over the interval $0 \leq U \leq 3$, for $N = 120$ and 240 (Fig. 4(e)).

One may relate the incommensurate phase to the doped Luttinger liquid inspired by the Kitaev-Hubbard model [37–39]. Even if the system is a nearly flat band, it still preserves a small dispersion. It therefore permits a low-energy expansion into right- and left-moving modes, providing the kinetic basis for a Luttinger-liquid description. The occupation of the B orbital at $U = 0.24$ is $\bar{n}_B = 0.43859$ corresponds to a doped orbital $\delta_B \equiv 1/2 - \bar{n}_B \simeq 0.06141$ relative to half filling. Together with the estimate $c_{\text{eff}} \simeq 1$, this motivates a phenomenological interpretation in terms of a doped Luttinger liquid. In a single-component spinless Luttinger description, the low-energy excitations are collective density fluctuations, known as the Friedel oscillations [40, 41]. To quantify the spatial decay of this density modulation, we fit the B -orbital occupation for different U to the finite-chain Friedel form, following from the open-boundary one-point function of the density vertex operator, as derived in Eq. (65) and Appendix D, Eq. (D12), of Ref. [42].

$$\begin{aligned} \langle n_{iB} \rangle &= n_{\text{bg}}(i) + \frac{A \cos(Qi + \phi)}{[d(i)]^{K_{\text{eff}}}}, \\ d(i) &= \frac{L+1}{\pi} \sin\left(\frac{\pi i}{L+1}\right), \end{aligned} \quad (13)$$

where K_{eff} is the Luttinger parameter, $L = N/3$ is the number of unit cells and $n_{\text{bg}}(i)$ includes a constant background. Doping the effective low-energy band away from a commensurate filling shifts Q away from its commensurate value and introduces a spatial mismatch in the corresponding umklapp term. When the density field remains unlocked, this mismatch suppresses commensurate density pinning at long distances, allowing an incommensurate density response in a gapless liquid [43]. For $N = 240$, and $U = 0.24$ fitting over $11 \leq i \leq 70$ yields $K_{\text{eff}} = 0.751$ (Fig. 5). Excluding between eight and fifteen unit cells at each boundary gives $K_{\text{eff}} \simeq 0.73$ – 0.80 . The decrease of K_{eff} with increasing U indicates a progressively slower spatial decay of the density-oscillation envelope within the Friedel ansatz. This trend is consistent with an enhanced tendency toward density ordering as repulsion increases. These results are compatible with a Friedel oscillation description with an effective exponent below unity.

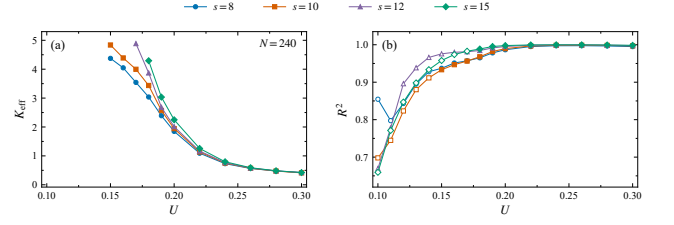


FIG. 5. Fitting the Luttinger parameter from the Friedel analysis Eq.(13) of the B -orbital density in the incommensurate regime, for $N = 240$ sites ($L = 80$ unit cells) and different fitting windows. (a) Effective exponent K_{eff} and (b) coefficient of determination R^2 versus U . Fits retain $s+1 \leq i \leq L-s$, with $s = 8, 10, 12, 15$ corresponding to the windows 9–72, 11–70, 13–68, and 16–65, respectively. Identical windows are used at every U .

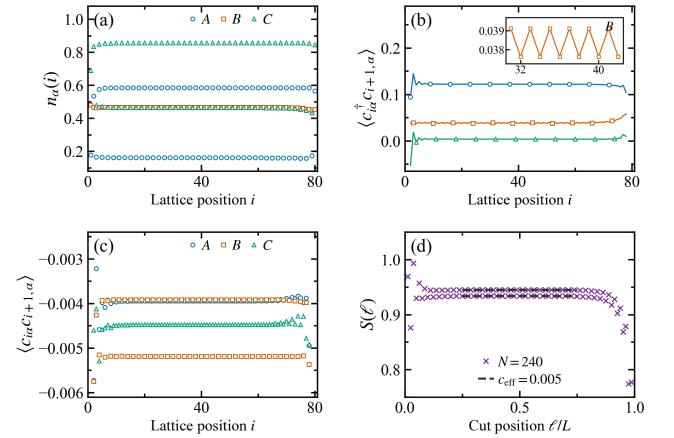


FIG. 6. Density, bond, pairing, and entanglement signatures of the intermediate CDW regime. (a) Orbital occupations $n_\alpha(i)$. (b) Normal bond expectation values (c) Pair expectation values $\langle c_{i\alpha} c_{i+1,\alpha} \rangle$. (d) Entanglement entropy at cell cuts ℓ , with $L = N/3 = 80$.

C. Regime III: intermediate CDW regime

The third regime is represented by $U = 0.50$ and $N = 240$. (Fig. 6(a)) shows a pronounced period-two density pattern on the A and C orbitals, while the B -orbital occupation remains nearly uniform in the bulk. To quantify this distinction, we define the staggered component of a local observable $O_\alpha(i)$ by

$$m_{O,\alpha} = \frac{1}{2} |\overline{O}_{\alpha,\text{even}} - \overline{O}_{\alpha,\text{odd}}|, \quad (14)$$

where the averages are taken separately over even and odd unit cells in the central half of the chain. The density amplitudes are $m_{n,A} = 0.2125$ and $m_{n,C} = 0.1964$, whereas $m_{n,B} \simeq 1.9 \times 10^{-6}$. The two large amplitudes vary by less than 0.2% between $N = 120$ and 240. These results support a commensurate AC -CDW pattern, with no comparable density staggering resolved on the B or-

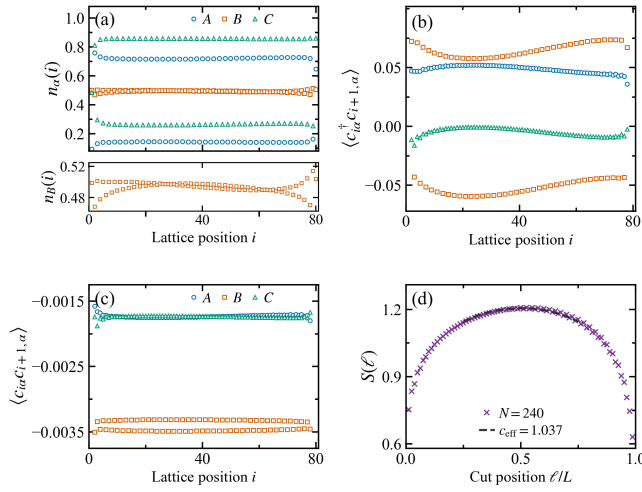


FIG. 7. Density, bond, pairing, and entanglement diagnostics of the second ICDW regime. (a) Orbital occupations $n_\alpha(i)$; the inset magnifies the unscaled B -orbital occupation over the full chain, with unit-cell position i on its horizontal axis. (b) Normal bond expectation values $\langle c_{i\alpha}^\dagger c_{i+1,\alpha} \rangle$. (c) Pair expectation values $\langle c_{i\alpha} c_{i+1,\alpha} \rangle$. (d) Entanglement entropy at unit-cell cuts ℓ , with $L = N/3 = 80$, giving $c_{\text{eff}} = 1.037$.

bital.

The bond and pairing profiles reveal a complementary orbital structure (Figs. 6(b) and (c)). For $B_\alpha(i) = \langle c_{i\alpha}^\dagger c_{i+1,\alpha} \rangle$ and $P_\alpha(i) = \langle c_{i\alpha} c_{i+1,\alpha} \rangle$, we obtain $m_{B,B} = 7.45 \times 10^{-4}$ and $m_{P,B} = 6.36 \times 10^{-4}$. The corresponding staggered components on A and C are below 10^{-6} . Thus, the B orbital supports alternating bond and pairing amplitudes despite its nearly uniform local density. The pairing modulation coexists with a nonzero uniform component, $\bar{P}_B = -0.00455$. The entanglement entropy approaches two nearly constant branches associated with even and odd cuts (Fig. 6(d)). Taken together, the profiles support a third regime with commensurate AC -CDW and B -orbital BOW/PDW modulations.

D. Regime IV: second ICDW regime

The fourth regime is represented by $U = 1.50$ and $N = 240$. The density profiles in (Fig. 7(a)) retain pronounced period-two components on the A and C orbitals. Defining the bulk staggered amplitude as $m_{O,\alpha} = |\bar{O}_{\alpha,\text{even}} - \bar{O}_{\alpha,\text{odd}}|/2$, we find $m_{n,A} = 0.2875$ and $m_{n,C} = 0.2970$. The strong density staggering thus remains concentrated on A and C , while the B channel develops a distinct, weaker density response.

The bond and pair expectation values show that the B -orbital modulations persist (Figs. 7(b) and (c)). For $B_\alpha(i) = \langle c_{i\alpha}^\dagger c_{i+1,\alpha} \rangle$ and $P_\alpha(i) = \langle c_{i\alpha} c_{i+1,\alpha} \rangle$, the staggered amplitudes are $m_{B,B} = 5.88 \times 10^{-2}$ and $m_{P,B} = 8.41 \times 10^{-5}$. Their counterparts on A and C are at most 1.8×10^{-4} and 1.4×10^{-6} , respectively. These data sup-

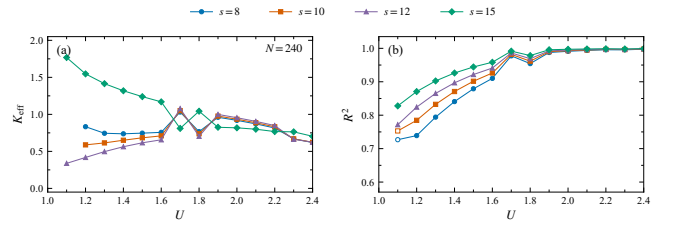


FIG. 8. Fitting the Luttinger parameter from the Friedel analysis Eq.(13) of the B -orbital density in the second incommensurate regime, for $N = 240$ sites ($L = 80$ unit cells) and different fitting windows. (a) Effective exponent K_{eff} and (b) coefficient of determination R^2 versus U . Fits retain $s + 1 \leq i \leq L - s$, with $s = 8, 10, 12, 15$ corresponding to the windows 9–72, 11–70, 13–68, and 16–65, respectively. Identical windows are used at every U .

port predominantly B -orbital BOW and PDW modulations coexisting with the AC -CDW background.

The decisive distinction from the third regime is the recovery of logarithmic entanglement scaling (Fig. 7(d)), with a fit over $20 \leq \ell \leq 60$ yielding $c_{\text{eff}} = 1.037$ for $N = 240$. In this regime, the spatially modulated B -orbital density is interpreted as an incommensurate charge-density-wave (ICDW) response, coexisting with commensurate CDW order on the A and C orbitals. As shown above (Fig. 4(e)), increasing U drives the average B -orbital occupation from a doped value toward half filling. Together with the evolution of the spatial profiles, this trend may suggest a sequence of commensurate-incommensurate (C-IC) transitions, reflecting competition between commensurate locking and a density modulation whose preferred wave vector evolves with the orbital occupation. Upon approaching half filling, commensurate locking becomes favored, and the B -orbital density develops a period-two CDW pattern. This interpretation relies on the density modulations as well as the occupation: the approach of $\bar{n}_B$ to $1/2$ alone does not establish the intermediate C-IC transitions.

We apply the same Friedel analysis to the B -orbital density in the fourth regime (Fig. 8). Compared with the second regime, the extracted exponent exhibits stronger window dependence over much of the interaction range. At $U = 1.5$, the primary window $11 \leq i \leq 70$ yields $K_{\text{eff}} = 0.683$, whereas the four windows give values between 0.616 and 1.239, indicating that a unique exponent is not reliably determined. More consistent fits emerge for $1.9 \leq U \leq 2.4$, where the primary-window exponent decreases from 0.977 to 0.624 and R^2 exceeds 0.99. Within the fitted ansatz, this decrease indicates a more slowly decaying density-oscillation envelope and is compatible with an enhanced tendency toward density ordering.

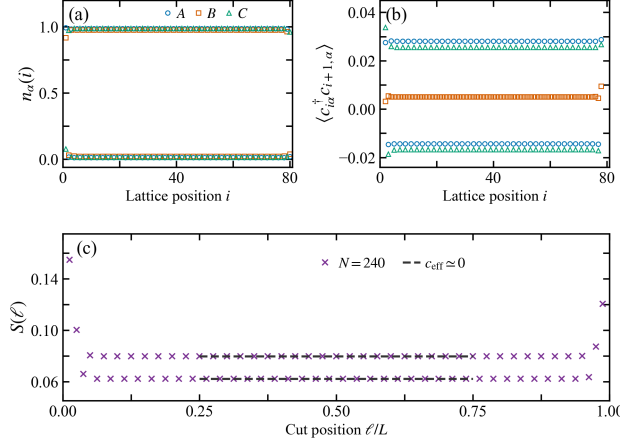


FIG. 9. Density, bond, and entanglement diagnostics of the strong coupling CDW phase. (a) Orbital occupations $n_\alpha(i)$. (b) Bond expectation values $\langle c_{i\alpha}^\dagger c_{i+1,\alpha} \rangle$. Colors and symbols distinguish A , B , and C in (a) and (b). (c) Entanglement entropy at unit-cell cuts, with $L = N/3 = 80$.

E. Regime V: strong-coupling CDW regime

The fifth regime is represented by $U = 5.0$ and $N = 240$. (Fig. 9(a)) shows pronounced period-two density modulations on all three orbitals. The bulk staggered amplitudes are $m_{n,A} = 0.4875$, $m_{n,B} = 0.4770$, and $m_{n,C} = 0.4876$, where $m_{O,\alpha} = |\bar{O}_{\alpha,\text{even}} - \bar{O}_{\alpha,\text{odd}}|/2$ is evaluated over $21 \leq i \leq 60$. The B orbital is nearly half filled, $\bar{n}_B = 0.500006$, with occupations alternating between approximately 0.9770 and 0.0230. Its approach to half filling is thus accompanied by strong commensurate density ordering. The entanglement entropy is correspondingly small, saturating at approximately 0.062 and 0.080 for odd and even bulk cuts, respectively (Fig. 9(c)). This weak entanglement is consistent with a state close to a classical charge configuration and, together with the pronounced density staggering. These results support an ABC -CDW phase.

The bond profiles reveal a predominantly AC -BOW component (Fig. 9(b)). For $B_\alpha(i) = \langle c_{i\alpha}^\dagger c_{i+1,\alpha} \rangle$, the staggered amplitudes on A and C are both approximately 2.12×10^{-2} , whereas the B -orbital amplitude is only 2.23×10^{-6} . The dominant bond modulation therefore shifts from B in the fourth regime to A and C in the fifth regime. The pair expectation values also retain weak spatial modulations, with amplitudes 9.77×10^{-7} and 1.30×10^{-6} on A and C . In this strong-coupling regime, the large intercell repulsion favors nearly classical charge configurations and suppresses pair fluctuations, making an independent PDW instability less likely. We therefore characterize this regime as an ABC -CDW state with predominantly AC bond modulation, without assigning an additional PDW order.

V. CONCLUSION AND REMARKS

We have investigated the interaction-driven evolution of the Lieb–Kitaev chain using orbital-resolved densities, bond and pairing expectation values, and entanglement entropy. The five finite-size regimes indicate how quantum geometry, orbital charge redistribution, and commensurate ordering shape the physics of an interacting nearly flat-band system. Their distinction requires resolving the individual orbitals, whose density and bond responses can evolve differently under the same interaction.

In the first regime, the bulk density remains spatially uniform within each orbital, and the entanglement entropy saturates with a negligible logarithmic contribution. The single-particle correlations decay exponentially, with a fitted decay length close to $4\xi_{\text{QM}}$ near the noninteracting limit, where ξ_{QM} is estimated from the underlying band geometry. This numerical agreement supports a quantum-geometric interpretation of the correlation length in the weakly interacting regime and connects the real-space correlations to the geometry of the nearly flat band.

Increasing the interaction produces a sequence of orbital-selective density reorganizations, accompanied by changes in entanglement scaling and bond modulation. Incommensurate density modulations first develop on all three orbitals in a critical regime compatible with $c_{\text{eff}} \simeq 1$. The A and C densities subsequently lock into period-two CDW patterns while the B density becomes nearly uniform, accompanied by entropy saturation and predominantly B -orbital bond modulation. A renewed incommensurate response then appears on B within the commensurate AC background, together with the recovery of logarithmic entanglement scaling. Finally, as the average B occupation approaches half filling, its density also locks into a period-two pattern, completing the ABC -CDW state. The small, saturated entropy in this strong-coupling regime supports a nearly classical charge configuration, while the dominant bond modulation shifts to A and C . The residual pairing modulation remains weak and does not establish an independent PDW phase in the presence of explicit pairing. Together, these observations suggest a competition between commensurate locking and incommensurate density responses, with distinct orbitals participating at different interaction strengths.

Future work should establish the thermodynamic transition boundaries through larger-system calculations, wave-vector scaling, and excitation-gap analysis. Pair-correlation and pairing-field studies could clarify the origin of the weak pairing response. Varying the residual bandwidth and orbital hybridization would further test how quantum geometry controls the correlation length and the subsequent sequence of orbital-selective ordering.

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